Spontaneous disentanglement of indistinguishable particles

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A master equation containing a nonlinear term that gives rise to disentanglement has been recently investigated. In this study, a modified version, which is applicable for indistinguishable particles, is proposed, and explored for both the Bose-Hubbard and the Fermi-Hubbard models. It is found for both Bosons and Fermions that disentanglement can give rise to quantum phase transitions.

**Introduction** - In standard quantum mechanics (QM), the time evolution of the density operator $\rho$ is governed by a master equation that has a linear dependency on $\rho$ [1]. A variety of nonlinear extensions to QM have been proposed [2–9]. These proposals have been mainly motivated by the old-standing problem of quantum measurement [10]. For some cases, the proposed extension can give rise to state vector spontaneous collapse [11–20]. Another motivation is related to the observation that dynamical instabilities [29] can be accounted for within the framework of standard QM [30]. For some cases, nonlinearity may give rise to conflicts with well-established physical principles, such as causality [31–36] and separability [32, 37, 38]. In addition, some predictions of standard QM, which have been experimentally confirmed to very high accuracy, are inconsistent with some of the proposed nonlinear extensions.

A nonlinear mechanism giving rise to suppression of entanglement (i.e. disentanglement) has been recently proposed [39]. This mechanism of disentanglement, which makes the collapse postulate redundant, is introduced by adding a nonlinear term to the master equation [see Eq. (2) below]. The proposed modified master equation can be constructed for any physical system whose Hilbert space has finite dimensionality, and it does not violate norm conservation of the time evolution. The nonlinear term added to the master equation has no effect on any product (i.e. disentangled) state. For a multipartite system, disentanglement between any pair of subsystems can be introduced by the added nonlinear term. Moreover, thermalization can be incorporated by an additional nonlinear term added to the master equation. The nonlinear extension that was proposed in [39] has been explored for systems containing distinguishable particles. The current work is devoted to disentanglement of indistinguishable particles. A modified master equation having a nonlinear term that generates disentanglement of indistinguishable particles is proposed. The dynamics generated by the proposed master equation is explored for both the Boson-Hubbard and the Fermi-Hubbard models [40–43].

**Indistinguishable particles** - The Hilbert space of a system containing indistinguishable particles can be constructed using a given orthonormal basis $\{|a_i\rangle\}$, that spans the single-particle Hilbert space $|\mathcal{H}\rangle$. The ket vector $|\vec{n}\rangle$ represents a state that is characterized by the vector $\vec{n} = (n_1, n_2, \ldots)$, where the integer $n_i$ is the number of particles that occupy the single particle state $|a_i\rangle$. The set $\{|\vec{n}\rangle\}$ forms an orthonormal basis for the many-particle Hilbert space. The state $|\vec{n}\rangle$ can be expressed in terms of the creation operators $a^\dagger_i$ as $|\vec{n}\rangle = (n_1, n_2, \ldots)^{-1/2} (a_1^\dagger)^{n_1} (a_2^\dagger)^{n_2} \cdots |0\rangle$, where $|0\rangle$ represents the state where all occupation numbers are zero. The number operator $N_i$ is defined by $N_i = a^\dagger_i a_i$.

It is postulated that the following commutation relations hold $[a_{i'}, a_{i''}]_+ = \delta_{i',i''}$ and $[a_{i'}, a_{i''}]_+ = \delta_{i',i''}$ for Fermions (Bosons), where $[A,B]_+ = AB \pm BA$ for general operators $A$ and $B$. For both Fermions and Bosons $N_i |\vec{n}\rangle = n_i |\vec{n}\rangle$. The relation $N_i = N_i^2$, which holds for Fermions, yields the Pauli’s exclusion principle. A single-particle unitary transformation mapping from the orthonormal basis $\{|a_i\rangle\}$ to an alternative orthonormal basis $\{|b_j\rangle\}$ yields the many-particle creation operator transformations given by $b_j^\dagger = \sum_i \langle a_i | b_j a_i^\dagger$, where $\langle a_i | b_j \rangle$ is the inner product of the single-particle states $|a_i\rangle$ and $|b_j\rangle$.

Observables of a system of identical particles must be defined in a way that is consistent with the principle of indistinguishability. Consider two-body interaction that is represented by a Hermitian operator $V_{TP}$ on the two-particle Hilbert space. A basis for this Hilbert space can be constructed using a given orthonormal basis for the single-particle Hilbert space $\{|b_j\rangle\}$. When the two particles are considered as distinguishable, the basis of the two-particle Hilbert space can be taken to be $\{|j', j''\rangle\}$. The ket vector $|j', j''\rangle$ represents a state, for which the first particle is in single particle state $|b_{j'}\rangle$, and the second one is in state $|b_{j''}\rangle$. Assume the case where the single-particle basis vectors $|b_j\rangle$ are chosen in such a way that diagonalizes $V_{TP}$, i.e. $V_{TP} |j', j''\rangle = v_{j', j''} |j', j''\rangle$, where the eigenvalue $v_{j', j''}$ is given by $v_{j', j''} = \langle j', j'' | V_{TP} |j', j''\rangle$. In the many-particle case, the two-particle interaction $V_{TP}$ is represented by

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the operator $V$, which for both Fermions and Bosons is given by

$$V = \frac{1}{2} \sum_{j',j''} v_{j',j''} N_{j'} \left( N_{j''} - \delta_{j',j''} \right), \quad (1)$$

where $N_j = b_j^\dagger b_j$. Note that the matrix element $\langle \bar{n} | V | \bar{n} \rangle$ is given by $\langle \bar{n} | V | \bar{n} \rangle = \sum_{j'<j''} n_j n_{j''} v_{j',j''} + (1/2) \sum_j n_j (n_j - 1) v_{j,j}$. While the factor $n_j n_{j''}$ represents the number of particle pairs occupying single-particle states $j'$ and $j''$ for the case $j' \neq j''$, the factor $n_j (n_j - 1)/2$ represents the number of particle pairs occupying the same single-particle state $j$. The expression given by Eq. (1) for the two-particle interaction in the basis that diagonalizes $V_{TP}$, is employed below for the construction of the nonlinear disentangling terms added to the master equation.

**Master equation** - The modified master equation for the density operator $\rho$ takes a form given by [6, 9, 18, 39, 45]

$$\frac{d\rho}{dt} = i\hbar^{-1} [\rho, H] - \Theta \rho - \rho \Theta + 2 \langle \Theta \rangle \rho, \quad (2)$$

where $\hbar$ is the Planck’s constant, $H = H^\dagger$ is the Hamiltonian, the operator $\Theta = \Theta^\dagger$ is allowed to depend on $\rho$, and $\langle \Theta \rangle = \text{Tr} (\Theta \rho)$. Note that $d\text{Tr} \rho/dt = 0$ provided that $\text{Tr} \rho = 1$ (i.e. $\rho$ is normalized), and that $d\text{Tr} \rho^2/dt = 0$, provided that $\rho^2 = \rho$ (i.e. $\rho$ represents a pure state).

For the case $H = 0$, and for a fixed operator $\Theta$, the expectation value $\langle \Theta \rangle$ monotonically decreases with time. Hence, the nonlinear term in the modified master equation (2) can be employed to suppress a given physical property, provided that $\langle \Theta \rangle$ quantifies that property. The operator $\Theta$ is taken to be given by $\Theta = \gamma_H Q^{(H)} + \gamma_D Q^{(D)}$, where both rates $\gamma_H$ and $\gamma_D$ are positive, and both operators $Q^{(H)}$ and $Q^{(D)}$ are Hermitian. The first term $\gamma_H Q^{(H)}$ gives rise to thermalization [46, 47], whereas disentanglement is generated by the second term $\gamma_D Q^{(D)}$.

Consider the master equation (2) for the case where $H$ is time independent, $\gamma_H = 0$ (i.e. no disentanglement), and $Q^{(H)} = \beta U_H$, where $U_H = H + \beta^{-1} \log \rho$ is the Helmholtz free energy operator, $\beta = 1/(k_B T)$ is the thermal energy density matrix, $k_B$ is the Boltzmann’s constant, and $T$ is the temperature. For this case, the thermal equilibrium density matrix $\rho_0$, which is given by $\rho_0 = e^{-\beta H}/\text{Tr} (e^{-\beta H})$, is a fixed-point steady state solution of the master equation (2), for which the Helmholtz free energy $\langle U_H \rangle$ is minimized [46–49]. The rate $\gamma_H$ represents the thermalization inverse time. The approximation $\langle U_H \rangle = \langle H \rangle$ can be employed in the low temperature limit.

**Two-particle disentanglement** - The disentanglement operator $Q^{(D)}$ is constructed based on the many-particle representation given by Eq. (1) for the two-particle interaction. Each term in Eq. (1) having the form $N_{j'} N_{j''}$ contributes to $Q^{(D)}$ a term given by $\eta_{j',j''} Q_{j',j''} (Q_{j',j''})^\dagger$, where

$$Q_{j',j''} = N_{j'} N_{j''} - \langle N_{j'} \rangle \langle N_{j''} \rangle. \quad (3)$$

A conflict with the causality principle [31–36] can be avoided, provided that the coefficients $\eta_{j',j''}$ (which are allowed to depend on $\rho$) are defined such that disentanglement generated by the operator $Q^{(D)}$ is active only when particles interact. However, for the below-discussed Hubbard model, it is assumed that $\eta_{j',j''} = 1$ (since nonlocality is irrelevant for this model with finite number of sites). Note that $\langle \bar{n} | Q^{(D)} | \bar{n} \rangle = 0$ for all basis vectors $| \bar{n} \rangle$ (provided that the many-particle basis states vectors $| \bar{n} \rangle$ are constructed based on a single-particle basis, for which the two-particle interaction $V_{TP}$ is diagonalized).

The relation $\Theta = \gamma_H Q^{(H)} + \gamma_D Q^{(D)}$ together with the ME (2) suggest that disentanglement can be accounted for by replacing the Helmholtz free energy $\langle U_H \rangle$ by an effective free energy $\langle U_E \rangle$, which is given by $\langle U_E \rangle = \langle U_H \rangle + \beta^{-1} \langle \gamma_H \rangle \langle Q^{(D)} \rangle$. For cases where the Hamiltonian $H$ is time-independent, the effective free energy $\langle U_E \rangle$ is locally minimized for fixed-point steady state solutions of the master equation (2).

Disentanglement is explored below for the one-dimensional Hubbard model [50]. In this model, indistinguishable particles occupy a one-dimensional array containing $L$ sites. The Hamiltonian $H$ is characterized by two real parameters, the nearest neighbor hopping coefficient $t$, and the on-site interaction coefficient $U$. The array is assumed to have a ring configuration, for which the first $l = 1$ and last $l = L$ sites are coupled. Some analytical results are derived below for the relatively simple case of two sites (i.e. $L = 2$).

**Bose-Hubbard model** - For the Bose-Hubbard model [51–53], the one-dimensional array is occupied by spinless Bosons. The creation and annihilation operators corresponding to site $l \in \{1, 2, \ldots, L \}$ are denoted by $b_l^\dagger$ and $b_l$, respectively. The operators $b_l^\dagger$ and $b_l$ satisfy Bosonic commutation relations. The Hamiltonian $H_B$ is given by

$$H_B = -t \sum_{l=1}^{L} \left( b_{l+1}^\dagger b_l + b_l b_{l+1}^\dagger \right) + \frac{U}{2} \sum_{l=1}^{L} N_l (N_l - 1), \quad (4)$$

where $N_l = b_{l+1}^\dagger b_l$. It is assumed that the array has a ring configuration, and thus, the last ($l = L$) hopping term $b_{L+1}^\dagger b_1 + b_1 b_{L+1}$ [see Eq. (4)] is taken to be given by $b_{L+1}^\dagger b_1 + b_1 b_{L+1}$. Note that the total number operator $N$, which is defined by $N = \sum_{l=1}^{L} N_l$, is a constant of the motion.

The linear part of the Hamiltonian $H_B$ (4) can be diagonalized using the transformation $b_l = L^{-1/2} \sum_{l'=1}^{L} e^{ik_l l'} a_{l'}$, where $k_l = 2\pi l/L$. In terms of the Bosonic creation and annihilation operators $a_l$ and $a_l^\dagger$, the condition $\langle N_l^2 \rangle = \langle N_l \rangle^2$ for all $l \in \{1, 2, \ldots, L \}$ is expressed as

$$\sum' \langle a_{l''}^\dagger a_l \rangle \langle a_{l''} a_l^\dagger \rangle = \sum' \langle a_{l''}^\dagger a_l \rangle \langle a_{l''} a_l^\dagger \rangle,$$

where the symbol $\sum'$ stands for summation over all $l''$, $l'''$, $l'''' \in \{1, 2, \ldots, L \}$ that satisfy the momentum conservation condition $l'' + l'''' = l + l'''$. For the case $L = 2$ (i.e. two sites), and
for the subspace of two Bosons (i.e. \(N = 2\)), the matrix representation of \(\mathcal{H}_B\) in the basis \(\{|n_2 = 0, n_1 = 2\}, |n_2 = 1, n_1 = 1\}, |n_2 = 2, n_1 = 0\}\) is given by

\[
\mathcal{H}_B = U \begin{pmatrix}
1 & -\tau & 0 \\
-\tau & 0 & -\tau \\
0 & -\tau & 1
\end{pmatrix},
\]  

(5)

where \(\tau = 2^{3/2}t/U\). The 3×3 Hamiltonian matrix \(\mathcal{H}_B\) (5) is diagonalized by the unitary matrix \(u\), which is given by

\[
u = \begin{pmatrix}
\frac{\sin \frac{\phi}{2}}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{\cos \frac{\phi}{2}}{\sqrt{2}} \\
-\cos \frac{\phi}{2} & 0 & \sin \frac{\phi}{2} \\
\frac{\sin \frac{\phi}{2}}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & \frac{\cos \frac{\phi}{2}}{\sqrt{2}}
\end{pmatrix},
\]  

(6)

where \(\tan \alpha = -2^{3/2} \tau\). The energy eigenvalues \(E_n\) are given by \(2E_1/U = 1 - \sqrt{1 + (8t/U)^2}\), \(E_2 = U\), and \(2E_3/U = 1 + \sqrt{1 + (8t/U)^2}\). For a density operator \(\rho\) having a 3×3 matrix representation given by

\[
\rho = \begin{pmatrix}
\cos^2 \frac{x + \frac{\pi}{2}}{2} & \cos^2 \frac{x}{2} & \cos^2 \frac{\phi}{2} \\
\sin^2 \frac{x}{2} & \sin^2 \frac{x + \frac{\pi}{2}}{2} & \sin^2 \frac{\pi}{2} \\
\sin^2 \frac{\phi}{2} & \sin^2 \frac{\phi}{2} & \sin^2 \frac{x}{2}
\end{pmatrix},
\]  

(7)

where \(x\) and \(\phi\) are real, and \(a\), \(b\) and \(c\) are complex, the energy expectation value \(\langle \mathcal{H}_B \rangle\) is given by \(\langle \mathcal{H}_B \rangle / U = \cos^2 \phi - \tau \text{Re}(a + b)\), and the following holds \((Q_{1,1}) = \langle Q_{2,2} \rangle = -\langle Q_{1,2} \rangle = (1 - \sin^2 (2x) \cos^2 \phi) \cos^2 \phi [\text{see Eq. (3)}]\).

For attractive interaction (i.e. \(U < 0\)), the ground state has energy \(E_0\) [the corresponding state vector is given by the third column of the unitary matrix \(u\) given by Eq. (6)]. In the absence of disentanglement (i.e. for \(\gamma_D = 0\)), and in the low temperature limit, the effective free energy \(\langle \mathcal{H} \rangle\) is locally minimized at the ground state. A stability analysis yields that, for the case \(|t/U| \ll 1\), a symmetry-breaking quantum phase transition occurs at \(-\gamma_D/(\beta U \gamma_T) \simeq 1/2\). This analytical result is validated by numerically integrating the master equation (2). The result is shown in Fig. 1, which depicts the dependency of \(\langle \mathcal{H}_B \rangle\) in steady state on \(-\gamma_D/(\beta U \gamma_T)\). The overlaid red dashed lines in Fig. 1 indicate the eigenvalues \(E_1\), \(E_2\) and \(E_3\).

**Fermi-Hubbard model** - For the Fermi-Hubbard model, the array is occupied by spin 1/2 Fermions. The Fermionic creation and annihilation operators corresponding to site \(l \in \{1, 2, \cdots, L\}\) with spin state \(\sigma \in \{\uparrow, \downarrow\}\) are denoted by \(b^\dagger_{l,\sigma}\) and \(b_{l,\sigma}\), respectively. The Hamiltonian \(\mathcal{H}_F\) is given by

\[
\mathcal{H}_F = -t \sum_{\sigma \in \{\uparrow, \downarrow\}} \sum_{l=1}^{L} (b^\dagger_{l,\sigma} b_{l+1,\sigma} + b^\dagger_{l+1,\sigma} b_{l,\sigma})
+ U \sum_{l=1}^{L} \left( N_{l,\uparrow} - \frac{1}{2} \right) \left( N_{l,\downarrow} - \frac{1}{2} \right),
\]  

(8)

where \(N_{l,\sigma} = b^\dagger_{l,\sigma} b_{l,\sigma}\). It is assumed that \(U > 0\) (i.e. interaction is repulsive). For \(\sigma \in \{\uparrow, \downarrow\}\), the total spin \(\sigma\) number operator \(N_\sigma\), which is defined by \(N_\sigma = \sum_{l=1}^{L} N_{l,\sigma}\), is a constant of the motion.

For the case \(L = 2\), the floor (lowest energy) state \(|f\rangle\) and the ceiling (highest energy) state \(|c\rangle\) of the Hamiltonian \(\mathcal{H}_F\) (8) are given by

\[
|f\rangle = \frac{(|0011\rangle + |1100\rangle) \cos \alpha + (|0110\rangle + |1001\rangle) \sin \alpha}{\sqrt{2}},
\]

(9)

\[
|c\rangle = \frac{(|0011\rangle + |1100\rangle) \sin \alpha - (|0110\rangle + |1001\rangle) \cos \alpha}{\sqrt{2}},
\]

(10)

where \(\alpha = (1/2) \tan^{-1}(-8t/U)\). The energy expectation value \(\langle \mathcal{H}_F \rangle\), which is calculated by numerically integrating the master equation (2), is plotted in Fig. 2 as a function \(\gamma_D/(\beta U \gamma_T)\). Both below and above the phase transition seen in Fig. 2, the occupation probabilities of all states, except of the floor \(|f\rangle\) and the ceiling \(|c\rangle\) ones, is found to be small (below \(10^{-5}\) for the range plotted in Fig. 2).

Consider a pure normalized state \(|\psi\rangle\) given by

\[
|\psi\rangle = e^{i\varphi} \cos(\varphi) |f\rangle + e^{-i\varphi} \sin(\varphi) |c\rangle,
\]

where
both $\phi$ and $\varphi$ are real. The following holds
\[
\langle \psi | H_F | \psi \rangle / U = -\cos (2\phi) / \cos (2\alpha) \quad \text{and} \quad \langle N_{1,\uparrow} N_{1,\downarrow} \rangle - \langle N_{1,\uparrow} \rangle \langle N_{1,\downarrow} \rangle = \langle N_{2,\uparrow} N_{2,\downarrow} \rangle - \langle N_{2,\uparrow} \rangle \langle N_{2,\downarrow} \rangle \equiv \nu, \quad \text{where} \quad \nu = (1/4) \cos (2\alpha) (\tan (2\alpha) \sin (2\phi) \cos (2\varphi) - \cos (2\phi)).
\]
In the absence of disentanglement (i.e. for $\gamma_D = 0$), and in the low temperature limit, the effective free energy $\langle U_e \rangle$ is locally minimized at the floor (ground) state $|f\rangle$. A stability analysis for the case $t/U \ll 1$ yields a symmetry-breaking quantum phase transition occurring at $\gamma_D / (\beta U \gamma_T) = 4$. This analytical result is validated by the plot shown in Fig. 2. The overlaid red dashed lines in Fig. 2 indicate the 16 energy eigenvalues of $H_F$.

**Discussion** - Below the phase transition (see Fig. 1 for Bosons, and Fig. 2 for Fermions), in steady state the ground state is nearly fully occupied (in the low-temperature limit). The disentanglement term added to the master equation (2) suppresses the expectation value $\langle Q^{(D)} \rangle$, which quantifies correlation between particles. For both above-discussed examples, the value of $\langle Q^{(D)} \rangle$ is not minimized at the ground state. Consequently, when the rate of disentanglement $\gamma_D$ is sufficiently large, occupying higher energy states becomes preferable, since that allows lowering the value of $\langle Q^{(D)} \rangle$.

The modified master equation given by Eq. (2) is by no means unique. Alternative mechanisms giving rise to disentanglement can be explored by redefining the operator $Q^{(D)}$. A variety of methods have been proposed to quantify entanglement of indistinguishable particles [54–59]. Some of these proposals can yield alternative definitions for the disentanglement operator $Q^{(D)}$. In the current study, the definition of the operator $Q^{(D)}$ is based on two-particle interaction [see Eq. (3)]. This chosen definition of $Q^{(D)}$ allows making disentanglement local (since disentanglement becomes active only when particles interact). In contrast, alternative definitions that enable remote disentanglement might give rise to a conflict with the causality principle [31–36].

The spontaneous disentanglement hypothesis is inherently falsifiable, because it yields predictions, which are experimentally distinguishable from predictions obtained from standard QM. For finite $L$, standard QM does not yield any phase transition in both Bose-Hubbard and Fermi-Hubbard models. On the other hand, phase transitions become possible when the mean field approximation is employed. For example, for the Fermi-Hubbard model, the mean field approximation yields a phase transition that occurs provided that the Stoner criterion is satisfied [60]. However, it has remained unclear how the mean field approximation, which is based on the assumption that entanglement can be disregarded, can be justified within the framework of standard QM. On the other hand, as is demonstrated by Figs. 1 and 2 for both Bosons and Fermions, in the presence of spontaneous disentanglement quantum phase transitions can occur in systems containing a finite number of particles.

**Summary** - Disentanglement of indistinguishable particles is explored. It is found for both Bosons and Fermions that disentanglement can give rise to quantum phase transitions, provided that the rate of disentanglement $\gamma_D$ is sufficiently large. Further study is needed to determine whether the hypothesis that spontaneous disentanglement occurs in quantum systems is consistent with experimental observations [61–64].


[46] H Grabert, “Nonlinear relaxation and fluctuations of


